

ABSTRACT OF THE INVENTION

NMR spectroscopy is increasingly used for the determination of the structure of proteins. According to the invention cross-signal pattern search masks are used for the joint evaluation of the 3D triple resonance experiments as well as the amino acid type-specific 2D spectra. All signal peaks due to an amino acid or a group of amino acids whose exact sequence has previously been derived from the protein sequence and forms the basis for the specific pattern recognition can be detected and evaluated jointly by means of pattern recognition with the aid of the cross-signal pattern search masks according to the invention. The invention permits a fully automated assignment of the signal peaks present in the various spectra to the magnetically active nuclei of the protein.